10 1701513

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1626rrw

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * *	* *	* *	* *	* Welcome to STN International * * * * * * * * *
NEWS	1			Web Page URLs for STN Seminar Schedule - N. America
NEWS	2			"Ask CAS" for self-help around the clock
NEWS	3	JAN	27	Source of Registration (SR) information in REGISTRY updated
				and searchable
NEWS	4	JAN	27	A new search aid, the Company Name Thesaurus, available in
				CA/CAplus
NEWS	5	FEB	05	German (DE) application and patent publication number format
				changes
NEWS	6	MAR	03	MEDLINE and LMEDLINE reloaded
NEWS	7	MAR	03	MEDLINE file segment of TOXCENTER reloaded
NEWS	8	MAR	03	FRANCEPAT now available on STN
NEWS	9	MAR	29,	Pharmaceutical Substances (PS) now available on STN
NEWS		MAR		WPIFV now available on STN
NEWS		MAR		New monthly current-awareness alert (SDI) frequency in RAPRA
 NEWS				PROMT: New display field available
NEWS	13	APR	26	IFIPAT/IFIUDB/IFICDB: New super search and display field
			_	available
NEWS				LITALERT now available on STN
NEWS		APR	27	NLDB: New search and display fields available
NEWS		May		PROUSDDR now available on STN
NEWS	17	May	19	PROUSDDR: One FREE connect hour, per account, in both May
MEMO	1.0	M	10	and June 2004
NEWS NEWS		May May		EXTEND option available in structure searching
NEWS		May		Polymer links for the POLYLINK command completed in REGISTRY FRFULL now available on STN
NEWS		May		STN User Update to be held June 7 and June 8 at the SLA 2004
MEMS	, 2 1	May	21	Conference
NEWS	22	May	27	New UPM (Update Code Maximum) field for more efficient patent
112112		r.a.y	2,	SDIs in Caplus
NEWS	23	May	27	CAplus super roles and document types searchable in REGISTRY
NEWS	_	May	27	Explore APOLLIT with free connect time in June 2004
NEWS	EXP	RESS	MAF	CH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
				CINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
				CURRENT DISCOVER FILE IS DATED 26 APRIL 2004
NEWS	HOUR	RS	STN	Operating Hours Plus Help Desk Availability
NEWS				eral Internet Information
NEWS	LOGI	N		come Banner and News Items
NEWS	PHON	ΙE	Dir	ect Dial and Telecommunication Network Access to STN
NEWS	WWW			World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 15:09:39 ON 17 JUN 2004

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 15:10:00 ON 17 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ${\tt ZIC/VINITI}$ data file provided by InfoChem.

STRUCTURE FILE UPDATES: 16 JUN 2004 HIGHEST RN 694434-66-7 DICTIONARY FILE UPDATES: 16 JUN 2004 HIGHEST RN 694434-66-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> isophoronenitrile/cn
ISOPHORONENITRILE IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> d

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 7027-11-4 REGISTRY

CN Cyclohexanecarbonitrile, 1,3,3-trimethyl-5-oxo- (7CI, 8CI, 9CI) (CA INDEX NAME)

OTHER NAMES:

CN 3-Cyano-3,5,5-trimethylcyclohexanone

CN 3-0xo-1,5,5-trimethylcyclohexanecarbonitrile

CN Isophoronenitrile

CN NSC 171143

```
10/458135
```

```
FS
     3D CONCORD
     144975-27-9, 78948-79-5
MF
     C10 H15 N O
     STN Files:
LC
                   BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMLIST,
       RTECS*, SPECINFO, TOXCENTER, USPAT2, USPATFULL
          (*File contains numerically searchable property data)
                       TSCA**
     Other Sources:
          (**Enter CHEMLIST File for up-to-date regulatory information)
       CAplus document type: Journal; Patent
       Roles from patents: BIOL (Biological study); FORM (Formation,
       nonpreparative); OCCU (Occurrence); PREP (Preparation); PROC (Process);
       RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
       Roles for non-specific derivatives from patents: PREP (Preparation);
       RACT (Reactant or reagent)
       Roles from non-patents: BIOL (Biological study); MSC (Miscellaneous); PREP (Preparation); RACT (Reactant or reagent); NORL (No role in record)
RL.NP
```

CN Me

Me

Me

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 88 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 88 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
- => s isophorone/cn L2 1 ISOPHORONE/CN => d

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN RN 78-59-1 REGISTRY CN 2-Cyclohexen-1-one, 3,5,5-trimethyl- (8CI, 9CI) (CA INDEX NAME) OTHER NAMES: CN α -Isophoron CN α -Isophorone

CN 1,1,3-Trimethyl-3-cyclohexene-5-one
CN 1,5,5-Trimethyl-3-oxocyclohexene
CN 1-Cyclohexen-3-one, 1,5,5-trimethylCN 3,5,5-Trimethyl-2-cyclohexen-1-one
CN 3,5,5-Trimethyl-2-cyclohexene-1-one
CN 3,5,5-Trimethyl-2-cyclohexene-1

CN 3,5,5-Trimethyl-2-cyclohexenone CN Isoacetophorone

CN Isoforon
CN Isophoron
CN Isophorone

10/458135

Page 4

CN NSC 403657

CN NSC 4881

FS 3D CONCORD

MF C9 H14 O

CI COM

LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DETHERM*, DIPPR*, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PDLCOM*, PIRA, PROMT, RTECS*, SPECINFO, TOXCENTER, ULIDAT, USPAT2, USPATFULL, VTB

(*File contains numerically searchable property data)

Other Sources: DSL**, EINECS**, TSCA**

RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)

RLD.P Roles for non-specific derivatives from patents: PREP (Preparation); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)

RLD.NP Roles for non-specific derivatives from non-patents: BIOL (Biological study); PREP (Preparation); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2503 REFERENCES IN FILE CA (1907 TO DATE)

20 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

2506 REFERENCES IN FILE CAPLUS (1907 TO DATE)

23 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file casreact
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 14.50 14.71

FULL ESTIMATED COST

FILE 'CASREACT' ENTERED AT 15:13:02 ON 17 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS) 10/458135

Page 5

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FILE CONTENT: 1840 - 13 Jun 2004 VOL 140 ISS 24

Some records from 1974 to 1991 are derived from the ZIC/VINITI data file and provided by InfoChem and some records are produced using some INPI data from the period prior to 1986.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Crossover limits have been increased. See HELP RNCROSSOVER for details.

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

Uploading C:\Program Files\Stnexp\Queries\10701513.str

L3 STRUCTURE UPLOADED

=> d

L3 HAS NO ANSWERS

L3

STR

Structure attributes must be viewed using STN Express query preparation.

≃> s L3

10/458135 Page 6 .

SAMPLE SEARCH INITIATED 15:13:41 FILE 'CASREACT'
SCREENING COMPLETE - 2 REACTIONS TO VERIFY FROM 2 DOCUMENTS

100.0% DONE 2 VERIFIED 0 HIT RXNS 0 DOCS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED VERIFICATIONS: 2 TO 124
PROJECTED ANSWERS: 0 TO 0

L4 0 SEA SSS SAM L3 (0 REACTIONS)

=> s L3 full

FULL SEARCH INITIATED 15:13:52 FILE 'CASREACT'

SCREENING COMPLETE - 8 REACTIONS TO VERIFY FROM 6 DOCUMENTS

0 HIT RXNS

0 DOCS

100.0% DONE 8 VERIFIED SEARCH TIME: 00.00.01

SEARCH TIME: 00.00.01

L5 0 SEA SSS FUL L3 (0 REACTIONS)

=> file caplus
COST IN U.S. DOLLARS

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 103.98 118.69

FILE 'CAPLUS' ENTERED AT 15:15:24 ON 17 JUN 2004
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FILE COVERS 1907 - 17 Jun 2004 VOL 140 ISS 25 FILE LAST UPDATED: 16 Jun 2004 (20040616/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 15:09:39 ON 17 JUN 2004)

FILE 'REGISTRY' ENTERED AT 15:10:00 ON 17 JUN 2004

L1 1 S ISOPHORONENITRILE/CN L2 1 S ISOPHORONE/CN

FILE 'CASREACT' ENTERED AT 15:13:02 ON 17 JUN 2004

```
10/458135
                                                                                     Page 7
L3
                 STRUCTURE UPLOADED
L4
               0 S L3
L5
               0 S L3 FULL
     FILE 'CAPLUS' ENTERED AT 15:15:24 ON 17 JUN 2004
=> s L1
Lб
             88 L1
=> s L2
           2508 L2
Ь7
=> s L6 and L7
             28 L6 AND L7
L8
    s L8 and (HCN or hydrogen cyanide)
         22796 HCN
         823229 HYDROGEN
          75403 CYANIDE
           8638 HYDROGEN CYANIDE
                   (HYDROGEN (W) CYANIDE)
             18 L8 AND (HCN OR HYDROGEN CYANIDE)
Ь9
=> s L9 and ?oxide
       2400861 ?OXIDE
              7 L9 AND ?OXIDE
L10
=> d L8 1-28 ibib abs
     ANSWER 1 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
                           2004:386596 CAPLUS
ACCESSION NUMBER:
                           140:391385
DOCUMENT NUMBER:
                           Regioselective hydrocyanation process for the calcium
TITLE:
                           oxide-catalyzed preparation of isophorone nitrile from
                           hydrogen cyanide and isophorone
                           Kunsmann-Keitel, Dagmar; Braun, Gerold; Muenster,
INVENTOR (S):
                           Ingo; Mundinger, Klaus; Scherhag, Gunter; Siegel,
                           Wolfgang
                           BASF Aktiengesellschaft,
                                                      Germany
PATENT ASSIGNEE(S):
                           Eur. Pat. Appl., 5 pp.
SOURCE:
                           CODEN: EPXXDW
DOCUMENT TYPE:
                           Patent
LANGUAGE:
                           German
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
     PATENT NO.
                        KIND DATE
                                               APPLICATION NO.
                                                                 DATE
         1418172 A2 20040512 EP 2003-25652 20031107
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     EP 1418172
     DE 10251680
                         A1
                              2Ø040519
                                              DE 2002-10251680 20021107
      JP 2004155785
                         A2
                               20040603
                                               JP 2003-375444
                                                                 20031105
                              20040513
                                                                  20031106
                                               US 2003-701513
     US 2004092761
                         Α1
                                           DE 2002-10251680 A 20021107
PRIORITY APPLN. INFO.:
     A regioselective hydrocyanation process for the calcium oxide-catalyzed
     preparation of isophorone nitrile from hydrogen cyanide and isophorone is
     presented in which the calcium oxide regioselective hydrocyanation
     catalyst has a BET surface area of >1.5 m2/g.
```

```
ACCESSION NUMBER:
                          2000:96029 CAPLUS
                          132:124501
DOCUMENT NUMBER:
TITLE:
                          Hydrocyanation process and catalyst for the
                          preparation of 3-cyano-3,5,5-trimethylcyclohexanone
                          from isophorone and hydrogen cyanide
INVENTOR(S):
                          Fischer, Jakob; Siegel, Wolfgang; Bomm, Volker;
                          Fischer, Martin; Mundinger, Klaus
PATENT ASSIGNEE(S):
                          BASF A.-G., Germany
                          U.S., 4 pp.
CODEN: USXXAM
SOURCE:
DOCUMENT TYPE:
                          Patent
LANGUAGE:
                          English
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
     PATENT NO.
                      KIND DATE
                                             APPLICATION NO. DATE
                     ----
     US 6022988
                     Α
                             20000208
                                            US 1999-372062 19990811
                                            DE 1998-19836474 19980812
     DE 19836474
                       Al
                             20000217
     EP 985659
                       A1
                             20000315
                                             EP 1999-115469
                                                             19990805
     EP 985659
                       B1
                             20031029
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
PRIORITY APPLN. INFO.:
                                          DE 1998-19836474 A 19980812
     3-Cyano-3,5,5-trimethylcyclohexanone is prepared in high yield and
     selectivity by reacting isophorone with hydrogen cyanide at 80-220°
     in the presence of the betaine catalyst 1,3-dimethylimidazolium-4-
     carboxylate.
REFERENCE COUNT: /
                          12
                                THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS
                                RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
     ANSWER 3 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
                          1999:662214 CAPLUS
ACCESSION NUMBER:
                          132:49772
DOCUMENT NUMBER:
                          Synthesis of 3H-labeled 2-hydroxy-N-[(1,3,3-trimethyl-
TITLE:
                          [4,5,6-3H]cyclohexyl)methyl]-5-azidobenzamide, a
                          photoaffinity analog of an influenza fusion inhibitor
                          Dischino, Douglas D.; Cianci, Christopher; Krystal, Mark; Meanwell, Nicholas A.; Morimoto, Hiromi; Pearce,
AUTHOR (S):
                          Bradley C.; Williams, Philip; Yu, Kuo-Long
CORPORATE SOURCE:
                          The Richard L. Gelb Center for Research and
                          Development, Bristol-Myers Squibb Company,
                          Wallingford, CT, 06492-7660, USA
                          Journal of Labelled Compounds & Radiopharmaceuticals
SOURCE:
                          (1999), 42(10), 965-974
CODEN: JLCRD4; ISSN: 0362-4803
PUBLISHER:
                          John Wiley & Sons Ltd.
DOCUMENT TYPE:
                          Journal
LANGUAGE:
                          English
     The title compound was prepared by tritiation of a mixture of
     N-(tert.-butoxycarbonyl)-1,3,3-trimethylcyclohex-4- and -5-enylmethylamine
     via T2 and Pd/C, followed by coupling of the deprotected tritiated \epsilon
     with 5-azidoacetylsalicylic acid chloride, followed by deprotection
     target compound was obtained with a radiochem. purity > 99% and a \epsilon
     activity of 63 Ci/mmol.
REFERENCE COUNT:
                                THERE ARE 14 CITED REFERENCES AVAILABLE
                                RECORD. ALL CITATIONS AVAILABLE IN THE
```

ANSWER 2 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ANSWER 4 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1995:907770 CAPLUS

DOCUMENT NUMBER:

123:313436

TITLE:

Process for the preparation of 3-cyano-3,5,5-

trimethylcyclohexanone [isophorone nitrile]

INVENTOR(S): Mundinger, Klaus; Laqua, Gerhard; Witzel, Tom; Merger, Franz

PATENT ASSIGNEE(S): SOURCE:

BASF A.-G., Germany Eur. Pat. Appl., 8 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 671384	A1	(1995)0913	EP 1995-102923	19950302
EP 671384	B1	199 91103		
R: BE, DE,	FR, G	3		
DE 4407487	A1	19950914	DE 1994-4407487	19940307
US 5516928	A	19960514	US 1995-395322	19950228
PRIORITY APPLN. INFO	. :	DI	E 1994-4407487	19940307
OTHER SOURCE(S):	CZ	ASREACT 123:3134	436; MARPAT 123:31	3436
GI				

AΒ The title compound (I), an intermediate for the monomer isophoronediamine, is prepared by a method using improved catalysts. Thus, isophorone (II) reacts with HCN to give I, at 80-180° and 0.5-20 bar, in the presence of an ammonium salt catalyst R1R2R3R4N+ X- [R1-R4 = C1-18 alkyl, C5-8 cycloalkyl, aryl, C7-18 aralkyl, C2-18 hydroxyalkyl; X = OCO2H, or OCO2R4 where R4 = C1-8 alkyl]. For example, a mixture of 3 mol HCN and 1.5mol II was added over 60 min to a mixture of 4.5 mol II and 30 mmol Me4N+ MeOCO2- at 120°. Acidification with 3.5 g 85% H3PO4 and distillation at 0.1 mbar gave I in 99% or 96.2% yield (based on unreacted II or fed HCN, resp.). In comparison, use of Et4N+ CN- catalyst gave 89.6% yield based on fed HCN. Also used as catalysts were BuMe3N+ MeOCO2-, and Et3MeN+ MeOCO2-, which gave similar results.

ANSWER 5 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1995:401307 CAPLUS

DOCUMENT NUMBER:

122:160152

TITLE:

Process for producing amines by reductive amination in

the presence of a cobalt catalyst.

INVENTOR(S):

Furutani, Atsushi; Hibi, Takuo; Yamamoto, Michio; Tanaka, Kazuyuki; Tada, Kazuhiro; Fukao, Masami;

Suzukamo, Gohfu

PATENT ASSIGNEE(S):

Sumitomo Chemical Co., Ltd., Japan

SOURCE:

Eur. Pat. Appl., 13 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent English

LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 623585	A1	19941109	EP 1994-300903	19940208
EP 623585 R: BE, DE,	B1 FR, GB	19980422		
JP 07101910	A2	19950418	JP 1994-6466	19940125
CA 2115024	AA	19941028	CA 1994-2115024	19940204
US 5589596	A	19961231	US 1994-194328	19940208
PRIORITY APPLN. INFO	. :		JP 1993-101074	19930427
			JP 1993-180248	19930721
			JP 1993-180249	19930721
			JP 1993-196041	19930806
			JP 1993-197339	19930809

OTHER SOURCE(S):

CASREACT 122:160152

A process is disclosed for producing amines by reductive amination of cyclic ketones or their imino derivs., characterized by use of a cobalt catalyst containing an alkaline earth metal carbonate and/or lanthanum oxide.

The

new catalysts give high yields, are highly active, and are usable on a com. scale. For example, an aqueous solution of Co and Cu nitrates was treated with Ca carbonate, heated to 80°, and treated with aqueous Na carbonate to give a precipitate, which was retreated with aqueous Na carbonate, dried,

heated

in N at 320°, cooled, granulated, and hydrogenated at 280° to give a catalyst. 3-Cyano-3,5,5-trimethylcyclohexanone was then passed with MeOH and liquid NH3 through a first reactor containing active C at 24° and 150 kg/cm2G to give the imine derivative in 97.7% yield. was passed through the above catalyst in a second reactor at 121° and the same pressure to give 3-aminomethyl-3,5,5-trimethylcyclohexylamine (I) in 99.4% yield, plus minor amts. of 2 byproducts. A comparison catalyst without the Cu nitrate or the Ca carbonate gave only 90.7% yield of I in the second step, with 5.8% 3-aminomethyl-3,5,5-trimethylcyclohexyl alc. and 3.2% 1,3,3-trimethyl-6-azabicyclo[3.2.1]octane as byproducts.

ANSWER 6 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1994:630393 CAPLUS

DOCUMENT NUMBER:

121:230393

TITLE:

Preparation of amines from cyclic ketones.

INVENTOR (S):

Furutani, Atsushi; Hibi, Takuo; Yamamoto, Michio;

Suzukamo, Gohfu

PATENT ASSIGNEE(S):

Sumitomo Chemical Company, Ltd., Japan

Eur. Pat. Appl., 7 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

SOURCE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 611137	A1	19940817	EP 1994-300915	19940208

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EP 611137
                     B1
                           19960424
       R: BE, DE, FR, GB
     JP 06285370
                    A2
                           19941011
                                         JP 1993-324532
                                                          19931222
                           19950829
    JP 07228562
                      A2
                                        JP 1994-303
                                                          19940106
                      AA
    CA 2115025
                           19940809
                                        CA 1994-2115025 19940204
    US 5395972
                     Α
                           19950307
                                         US 1994-194329
                                                          19940208
PRIORITY APPLN. INFO.:
                                       JP 1993-20134
                                                          19930208
                                      JP 1993-319593
                                                          19931220
OTHER SOURCE(S):
                        CASREACT 121:230393
    Cyclic ketones were reacted with NH3 in the presence of active C to
    produce imino derivs. which were reacted with H in the presence of a
    hydrogenation catalyst to give the corresponding amines. Thus,
     3-cyano-3,5,5-trimethylcyclohexanone, MeOH, and NH3 were fed to the first
    of a series of 2 connected reactors and H was added to the second reactor;
    the first packed with active C and the second packed with Co on silica.
    The temperature of the first reactor was 20° and that of the second was
     114°; reactor pressure was 70 kg/cm2G. Product
     3-aminomethyl-3,5,5-trimethylcyclohexylamine was formed in 94.9% yield.
    ANSWER 7 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:
                        1994:511943 CAPLUS
DOCUMENT NUMBER:
                        121:111943
TITLE:
                        Purification of 3-cyano-3,5,5-trimethyl-1-
                        cyclohexanone
INVENTOR(S):
                        Terasawa, Shoichi; Yamamoto, Masahiro
PATENT ASSIGNEE(S):
                        Asahi Chemical Ind, Japan
                        Jpn. Kokai Tokkyo Koho, 7 pp.
SOURCE:
                        CODEN: JKXXAF
DOCUMENT TYPE:
                        Patent
LANGUAGE:
                        Japanese
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
    PATENT NO.
                   KIND DATE
                                        APPLICATION NO. DATE
     -----
                          -----
                                         JP 1992-225631
                     A2 19940308
    JP 06065183
                                                          19920825
PRIORITY APPLN. INFO.:
                                     JP 1992-225631
                                                          19920825
    The title compound (I), prepared by the base-catalyzed addition reaction of HCN
    with isophorone, is purified by adding an inert compound having a higher
    b.p. than I and compatible with I, removing the basic catalyst,
    high-boiling impurities, and the inert compound in a thin-film evaporator,
    and separating isophorone from I in a distillation column. A reaction product
(180
    g) containing isophorone 18.02, I 80.9, high-boiling impurities 1.0, and NaOH
     0.08% was mixed with 3 g polyethylene glycol (II; mol. weight 400) and fed to
    a thin-film evaporator to give 177.3 g fraction containing 18.2% isophorone
    and 81.8% I (for separation by distillation) and 5.7 g fraction containing II
53,
    isophorone 3, and I 10%.
    ANSWER 8 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:
                        1994:511942 CAPLUS
DOCUMENT NUMBER:
                        121:111942
TITLE:
                        Purification of 3-cyano-3,5,5-trimethyl-1-
                        cyclohexanone
INVENTOR(S):
                        Terasawa, Shoichi; Kondo, Yoshikimi
PATENT ASSIGNEE(S):
                        Asahi Chemical Ind, Japan
SOURCE:
                        Jpn. Kokai Tokkyo Koho, 4 pp.
```

CODEN: JKXXAF

DOCUMENT TYPE:

Patent Japanese

LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

APPLICATION NO. DATE KIND DATE PATENT NO. ---------_____ ______ JP 06065182 A2 19940308 JP 1992-215834 19920813 JP 1992-160927 19920619 PRIORITY APPLN. INFO.:

The title compound (I), prepared by the alkali-catalyzed addition reaction of AB

with isophorone is purified by neutralizing the catalyst with an acid and distilling the mixture A reaction mixture containing I 60.5, isophorone 38, and KOH

0.30 mol was neutralized with H2SO4 and distilled (540 parts) in vacuo to give 226 parts distillate containing 12.7% I and 87.3% isophorone and 286 parts crystalline fraction containing 99.5% I.

L8

ANSWER 9 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1993:670685 CAPLUS

DOCUMENT NUMBER:

119:270685

TITLE:

Process for the continuous preparation of

3-cyano-3,5,5-trimethylcyclohexanone

INVENTOR (S):

Pander, Hans Joachim; Siegel, Hardo; Woerz, Otto

PATENT ASSIGNEE(S): SOURCE:

BASF A.-G., Germany Eur. Pat. Appl., 6 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

LANGUAGE:

Patent German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO. DATE
EP 554786	A1	19930811	EP 1993-101250 19930128
EP 554786	B1	19951129	
R: BE, DE,	FR, GB	, NL	
DE 4203456	A1	19930812	DE 1992-4203456 19920207
US 5254711	A	19931019	US 1993-14171 19930205
JP 06122667	A2	19940506	JP 1993-18562 19930205
JP 3241472	B2	20011225	
RITY APPLN. INFO	.:		DE 1992-4203456 A 19920207

PRIOR

OTHER SOURCE(S):

CASREACT 119:270685

The title process comprises condensation of isophorone with HCN in a 2-stage flow reactor system comprising an initial stage wherein complete mixing is provided and a second stage wherein mixing is suppressed. Thus, operation at 150° in both stages gave 96.5% the title compound

ANSWER 10 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1993:652567 CAPLUS

DOCUMENT NUMBER:

119:252567

TITLE:

Process for the preparation of 3-cyano-3,5,5-

trimethylcyclohexanone

Woodbury, Richard P.; Thunberg, Jon C.; Vankouwenberg, Steven P.; Begonis, Walter B. Hampshire Chemical Corp., USA

PATENT ASSIGNEE(S): SOURCE:

U.S., 10 pp.

CODEN: USXXAM

DOCUMENT TYPE:

INVENTOR (S):

Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA'	TENT NO.	KII	ND DATE		APPLICATIO	ON NO.	DATE
US	5235089	. A	1993	0810	US 1992-84	13867	19920227
AU	9333783	A:	1 1993	0902	AU 1993-33	3783	19930225
AU	660765	B	2 1995	0706			
CA	2090555	Ai	A 1993	0828	CA 1993-20	90555	19930226
EP	558332	A:	1993	0901	EP 1993-30	1451	19930226
EP	558332	B	1 1996	0529			
	R: AT,	BE, CH,	DE, DK,	ES, FR,	GB, IT, LI,	NL, PT,	SE
JP	06016612	A:	2 1994	0125	JP 1993-61	L314	19930226
AT	138642	E	1996	0615	AT 1993-30	1451	19930226
ES	2088225	T	3 1996	0801	ES 1993-30	1451	19930226
PRIORIT	Y APPLN.	INFO.:		υ	JS 1992-84386	57	19920227
_							

AB The title process giving title compound with high yield and low impurity comprises reacting isophorone with HCN in the presence of LiCN catalyst at 80-115° while maintaining the HCN at a controlled rate (to prevent the generation of free LiOH, diisophorone, its nitrile derivs., and HCN polymer); and adding an acid selected from malic acid, oxalic acid, sulfuric acid, and phosphoric acid to precipitate the Li salt.

L8 ANSWER 11 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1993:233534 CAPLUS

DOCUMENT NUMBER:

118:233534

TITLE:

Catalyst and process for the production of

3-cyano-3,5,5-trialkylcyclohexanone

Forguy, Christian; Goetz, Frederick J.; Graeber,

Edward L.; Lindstrom, Michael J.

PATENT ASSIGNEE(S):

Elf Atochem North America, Inc., USA

SOURCE:

U.S., 4 pp. CODEN: USXXAM

DOCUMENT TYPE:

INVENTOR (S):

Patent

LANGUAGE:

English

1

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5183915	A	19930202	US 1992-846364	19920305
EP 558799	A2	19930908	EP 1992-117471	19921013
EP 558799	A3	19950215		
R: AT, BE,	CH, DE	, DK, ES,	FR, GB, GR, IE, IT, LI	, LU, NL, PT, SE
CA 2080646	AA	19930906	CA 1992-2080646	19921015
JP 05294918	A2	19931109	JP 1992-314450	19921030
CN 1075954	A	19930908	CN 1992-112660	19921103
PRIORITY APPLN. INFO	. :		US 1992-846364	19920305
OTHER SOURCE(S):	MA	RPAT 118:2	233534	

AB Title compound is prepared by reaction of 3,5,5-tris(C1-4 alkyl)cyclohexanone with HCN in the absence of H2O and in the presence of quaternary ammonium-or phosphonium cyanide catalyst at 900-120° and 1-3 bar pressure. Isophorone and Et4N+CN- was heated to 105° followed by addition of HCN after which the temperature was increased to 112° and kept at 1102 for 1 h with stirring to give 3-cyclohexa-3,5,5-trimethylcyclohexanone.

L8 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 1993:59336 CAPLUS

DOCUMENT NUMBER:

118:59336

TITLE: INVENTOR (S): Preparation of 3-cyano-3,5,5-trimethylcyclohexanone Tabei, Nobuaki; Mizuno, Tadashi; Okamura, Haruki

PATENT ASSIGNEE(S):

Sumitomo Chemical Co., Ltd., Japan

SOURCE:

Jpn. Kokai Tokkyo Koho, 3 pp.

CODEN: JKXXAF

DOCUMENT TYPE: LANGUAGE:

Patent Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.

KIND DATE JP 04253948 A2 19920909 APPLICATION NO. DATE

JP 1991-15229 19910206 -----

PRIORITY APPLN. INFO.:

JP 1991-15229

OTHER SOURCE(S):

CASREACT 118:59336; MARPAT 118:59336

The title compound (I) is prepared by treating isophorone (II) with HCN in the presence of R2N:C(NR12)2 (III; R1, R2 = H, C1-4 alkyl). A mixture of II and III (R1 = Me, R2 = H) was treated dropwise with HCN at 105° over 3

h, then settled at 105° for 0.5 h to give 90.6% I.

ANSWER 13 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1993:21969 CAPLUS

DOCUMENT NUMBER:

118:21969

TITLE: INVENTOR(S): Preparation of 3-cyano-3,5,5-trimethylcyclohexanone

Terasawa, Shoichi; Yamamoto, Tadatsugu PATENT ASSIGNEE(S): Asahi Chemical Industry Co., Ltd., Japan

SOURCE:

Jpn. Kokai Tokkyo Koho, 3 pp. CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

KIND DATE

APPLICATION NO. DATE

-----JP 04279558

---------A2 19921005 JP 1991-4451 19910118 19910118

PRIORITY APPLN. INFO.:

PATENT NO.

JP 1991-4451

The title compound (I) is prepared by treating isophorone with HCN in the presence of basic catalysts and water. A mixture of isophorone and aqueous NaOH

was treated dropwise with HCN, then stirred at 170° to give I in 100% selectivity at 47.6% conversion.

ANSWER 14 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1992:570855 CAPLUS

DOCUMENT NUMBER: TITLE:

117:170855

Preparation of 3-cyano-3,5,5-trimethylcyclohexanone

INVENTOR (S): PATENT ASSIGNEE(S):

Terasawa, Shoichi; Yamamoto, Tadatsugu Asahi Chemical Industry Co., Ltd., Japan

SOURCE:

Jpn. Kokai Tokkyo Koho, 3 pp.

DOCUMENT TYPE:

CODEN: JKXXAF Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

KIND DATE

APPLICATION NO. DATE

PATENT NO.

JP 04164057 A2 19920609 JP 1990-285816 19901025 PRIORITY APPLN. INFO.: JP 1990-285816 19901025 CASREACT 117:170855 OTHER SOURCE(S): The title compds. (I), useful as material for 1-amino-3-aminomethyl-3,5,5trimethylcyclohexane and 1-isocyanato-3-(isocyanatomethyl)-3,5,5trimethylcyclohexane, is prepared by treating isophorone (II) with HCN in 1,3-dimethyl-2-imidazolidinone (III) in the presence of basic catalysts. A mixture of II and K2CO3 in III was treated dropwise with HCN at 110° over 4 h, then treated at 110° for 1 h to give I in 94% selectivity at 88% conversion.

ANSWER 15 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1992:492650 CAPLUS

DOCUMENT NUMBER:

117:92650

TITLE:

Manufacture of 3-cyano-3,5,5-trimethylcyclohexanone

INVENTOR(S): PATENT ASSIGNEE(S): Terasawa, Shoichi; Yamamoto, Tadatsugu Asahi Chemical Industry Co., Ltd., Japan

SOURCE:

Jpn. Kokai Tokkyo Koho, 3 pp.

DOCUMENT TYPE:

CODEN: JKXXAF Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE ----_____ -----JP 1990-232491 JP 04112862 19920414 19900904 A2 PRIORITY APPLN. INFO.: JP 1990-232491 19900904

Title compound (I) is manufactured from isophorone and HCN at 60-160° in Me2SO and/or DMF over a base catalyst. Thus, treating 1 mol isophorone with 1 mol HCN in Me2SO in the presence of K2CO3 at 110° gave 85% I vs. 41% in ethylene glycol.

ANSWER 16 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1992:425974 CAPLUS

DOCUMENT NUMBER:

117:25974

TITLE:

Preparation of bis-(3-cyano-3,5,5-

trimethylcyclohexylidene) azine and its conversion to

3-(aminomethyl)-3,5,5-trimethylcyclohexylamine

INVENTOR (S):

Huthmacher, Klaus; Schmitt, Hermann

PATENT ASSIGNEE(S):

Degussa A.-G., Germany

Eur. Pat. Appl., 11 pp.

SOURCE:

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PAT	CENT NO.		KIND	DATE		APPLICATION NO.	DATE
EP	482347		A2	19920429		EP 1991-115713	19910917
EP	482347		A3	19920819			
EP	482347		B1	19930609			
	R: AT,	BE,	CH, DE	, ES, FR,	GB,	IT, LI, NL	
DE	4033609		A1	19920507		DE 1990-4033609	19901023
DE	4033609		C2	19920910			
DE	4119577		A1	19921217		DE 1991-4119577	19910614
AT	90335		E	19930615		AT 1991-115713	19910917
ES	2059008		T3	19941101		ES 1991-115713	19910917

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JP 1991-273630
                      A2 19920918
                                                            19911022
     JP 04264057
                                           US 1991-785323
                                                            19911023
     US 5166396
                      A
                            19921124
                                           US 1992-848390
    US 5166444
                       Α
                            19921124
                                                            19920309
PRIORITY APPLN. INFO.:
                                        DE 1990-4033609
                                                            19901023
                                        DE 1991-4119577
                                                            19910614
                                                            19910917
                                        EP 1991~115713
                                        US 1991~785323
                                                            19911023
```

OTHER SOURCE(S): CASREACT 117:25974

The title azine, prepared in 92.7% yield from 1,3,3-trimethyl-5oxocyclohexanecarbonitrile and N2H4 in MeOH, was hydrogenated in MeOH-NH3 in the presence of Raney Ni and CoCl2 to give 91.2% title amine.

ANSWER 17 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1991:514033 CAPLUS

DOCUMENT NUMBER:

115:114033

TITLE:

Process for the preparation of 1,3,3-trimethy1-5-oxo-

cyclohexanecarbonitrile

INVENTOR(S):

Huthmacher, Klaus; Schmitt, Hermann

PATENT ASSIGNEE(S): SOURCE:

Degussa A.-G., Germany Eur. Pat. Appl., 7 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION: ______

	PATENT NO.		DATE		APPLICATION NO.	DATE		
		A1	19910626		EP 1990-120672	19901029		
	EP 433615 R: BE, CH, I		FR, GB,					
	DE 3942371 DE 3942371	A1 C2	19910627 19920521		DE 1989-3942371	19891221		
	ES 2060893	Т3	19941201			19901029		
						19901205 19901217		
	JP 07091256	B4	19951004		CA 1990-2032667	10001210		
	CA 2032667 CA 2032667				CA 1990-2032667	19901219		
	RITY APPLN. INFO.		SPEACT 115		DE 1989-3942371	19891221		
AB								
	the presence of	an alka	ali compou	nd	(LiOH) as catalyst a	HCN to isophorone in at 100-160°;	1	
	0.0005-5 mol% ca	talyst	are used	wit]	n resp. to isophorom	ne. HCN (40.5 g)		

was added to a mixture of isophorone (345 g) and LiOH (0.8 g) at 135° to give 89.1% I.

ANSWER 18 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1991:470990 CAPLUS

DOCUMENT NUMBER:

115:70990

TITLE:

Process for the preparation of 3-cyano-3,5,5-

trimethylcyclohexanone by addition of hydrogen cyanide

to isophorone

INVENTOR(S):

Thunberg, Jon C.; Begonis, Walter B.

PATENT ASSIGNEE(S):

W. R. Grace and Co., USA

SOURCE:

U.S., 7 pp. CODEN: USXXAM

DOCUMENT TYPE:

Patent

10/458135

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

KIND DATE APPLICATION NO. DATE PATENT NO. US 1990-475051 19900206 CA 1991-2034640 19910121 ----_____ A AA A 19910430 US 5011968 CA 2034640 19910807 PRIORITY APPLN. INFO.: US 1990-475051 19900206 The title compound (I), i.e. isophorone nitrile, is prepared by (a) reacting isophorone (II) with HCN in the presence of a quaternary ammonium hydroxide in a molar ratio of II:HCN:catalyst of (.apprx.2.00-3.00):1.00:(0.005-0.01) at a least 110°; (b) decomposing the remaining catalyst by heating the reaction mixture at .apprx.110-150°; (c) sparging with an inert gas at 100-200° to remove the catalyst decomposition product) and (d) acidifying the mixture with an acid and sparging with an inert gas to eliminate residual HCN. Thus, 172 lb II was charged via vacuum to a reactor of an apparatus (illustrated therein), N was introduced to break the vacuum, II was heated to 110°, 1.11 lb of 25% aqueous Me4N+OH- was added, and HCN was added, and the reaction was allowed to

L8 ANSWER 19 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1991:448914 CAPLUS

DOCUMENT NUMBER:

115:48914

TITLE:

Preparation of 3-cyano-3,5,5'-trimethyl-1-

cyclohexanone from isophorone and an alkaline cyanide

Page 17 '.

Pontoglio, Enrico; Parodi, Sandro

INVENTOR(S):

PATENT ASSIGNEE(S): SOURCE:

Caffaro S.p.A., Italy Eur. Pat. Appl., 5 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT:

proceed to give I.

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 425806	A1	19910508	EP 1990-117995	19900919
EP 425806	B1	19940601		
R: CH,	DE, ES, FR,	LI, NL		
ES 2054185	Т3	19940801	ES 1990-117995	19900919
US 5142090	A	19920825	US 1990-585240	19900920
JP 03153656	A2	19910701	JP 1990-298751	19901102
PRIORITY APPLN.	NFO.:	J	T 1989-22246	19891102

AB The title compound (I), which is used as a hardener for epoxy resins and as a monomer for polyurethane and polyamide resins, is prepared by reaction of isophorone (II) with an equivalent amount of an alkaline cyanide in a homogeneous

water/organic solvent solution at 20° to reflux temperature while maintaining a pH between 14-8 by a gradual addition of an inorg. acid during the reaction. Thus, II 553, DMF 600, and an aqueous NaCN 600 parts were heated at 90-92° with stirring while adding 85% H3PO4 and after 2 h the feeding of the acid was stopped and the temperature was raised to 104-105° allowing the reaction to complete for another 2 h. The reaction mixture was brought to pH 5.,5 with 85% H3PO4 and the upper layer containing I was removed and then distilled on a Vigreux column to give 78% I

of

97% purity.

ANSWER 20 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

1989:439343 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 111:39343

Applications of phase-transfer catalysis. Part 45. TITLE:

Enantioselective phase-transfer catalysis by optically

active crown ethers

Dehmlow, Eckehard V.; Sauerbier, Christiane AUTHOR (S):

Fak. Chem., Univ. Bielefeld, Bielefeld, D-4800/1, Fed. CORPORATE SOURCE:

Rep. Ger.

Journal

Liebigs Annalen der Chemie (1989), (2), 181-5 SOURCE:

CODEN: LACHDL; ISSN: 0170-2041

DOCUMENT TYPE:

LANGUAGE: German

CASREACT 111:39343 OTHER SOURCE(S):

GI

CH₂OR CH2OR Ι

AB Chiral crown ethers I (R = H, R1CO; R1 = Ph, substituted Ph) were prepared as chiral phase-transfer catalysts. I induced asymmetry in the epoxidn. of alkenones and in their reaction with HOCMe2CN. The maximum enantiomeric excess, 45%, was obtained in the reaction of (E)-PhCH:CHCOPh with HOCMe2CN in the presence of I (R = 2,4-Cl2C6H3CO).

ANSWER 21 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

1987:190539 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 106:190539

TITLE: Guinea pig pulmonary response to sensitization by five

preformed monoisocyanate-ovalbumin conjugates

AUTHOR (S): De Ceaurriz, Jacques; Ducos, Philippe; Micillino, Jean

Claude; Gaudin, Rene; Cavelier, Claude

Inst. Natl. Rech. Sec., Vandoeuvre, 54500, Fr. CORPORATE SOURCE:

SOURCE: Toxicology (1987), 43(1), 93-101

CODEN: TXCYAC; ISSN: 0300-483X

DOCUMENT TYPE: Journal

English LANGUAGE: GI

Me CH2NCO Me Me Ι

The ability of 5 dissimilar monoisocyanates conjugated to ovalbumin (OA) as a carrier protein to induce pulmonary hypersensitivity towards the hapten specific component was assessed by using a previously described

10/458135 Page 19

method based on the determination of a respiratory index (RI) in the guinea pig.

The test chemical included p-tolyl [622-58-2] and hexylmonoisocyanate [2525-62-4] (TMI and HMI), 4-isocyanatodiphenylmethane (IDM) [1823-37-6], 4-isocyanato-4'-methyldiphenylmethane (IMDM) [107997-84-2], and 1-isocyanatomethyl-1,3,3-trimethylcyclohexane (IMTC)(I) [107997-85-3]. Guinea pigs were exposed daily to an aerosol of the OA conjugate of each monoisocyanate up to ≤15 days. Increases in respiratory rate and/or respiratory collapse occurred in the guinea pigs exposed to TMI-OA and HMI-OA conjugates by days 9 and 15, with RI values of 155 and 177, resp.. The greatest mean RI values in guinea pigs exposed to IDM-OA, IMDM-OA, and IMTC-OA conjugates to day 15 were 20, 25, and 22, resp., and were not indicative of any pulmonary reaction. Guinea pigs exposed in parallel to each test conjugate did not exhibit any pulmonary reaction when they were exposed to OA on the challenge days. All these findings evidence pulmonary hypersensitivity as the result of exposure to TMI-OA and HMI-OA conjugates and suggest a high degree of conjugation and strong linkage of all the monoisocyanates with OA. The difference between the number of days to the onset of pulmonary reaction to TMI-OA and HMI-OA conjugates, and the lack of pulmonary reaction to IDM-OA, IMDM-OA, and IMTC-OA conjugates within the exptl. period suggest the influence of the nature of the haptenic portion on the lapse of time required for pulmonary response to OA preformed conjugates and point to the possibility of discriminating between the allergenic potential of the test materials on this basis.

ANSWER 22 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1986:442383 CAPLUS

DOCUMENT NUMBER:

105:42383

TITLE:

3-Cyano-3,5,5-trimethylcyclohexanone

INVENTOR(S):

Kondo, Kenji; Kosai, Hiroshi; Shidara, Hideo Nippon Chemicals Co., Ltd., Japan

PATENT ASSIGNEE(S): SOURCE:

Jpn. Kokai Tokkyo Koho, 5 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent. LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61033157	A2	19860217	JP 1984-153231	19840725
JP 05033217	B4	19930519		
PRIORITY APPLN. INFO.	:		JP 1984-153231	19840725

CASREACT 105:42383 OTHER SOURCE(S):

The title compound (I), useful as epoxy resin hardener, material for elastomers, polyurethane paints, etc. (no data), was prepared by reaction of isophorone (II) and HCN over quaternary ammonium hydroxide or quaternary phosphonium hydroxide. Thus, HCN was added dropwise to mixture of II, Bu4NOH, and H2O with stirring at 110° for 3 h and the resulting mixture allowed to stand at 110° for 1 h to give 94.9% I based on HCN.

ANSWER 23 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

1986:442382 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 105:42382

3-Cyano-3,5,5-trimethylcyclohexanone

Kondo, Kenji; Kosai, Hiroshi; Shidara, Hideo INVENTOR(S):

PATENT ASSIGNEE(S): Nippon Chemicals Co., Ltd., Japan

SOURCE:

Jpn. Kokai Tokkyo Koho, 4 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent Japanese

LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE ----______ 19860217 JP 61033158 A2 JP 1984-153233 19840725 19921224 JP 04081583 B4

PRIORITY APPLN. INFO.:

JP 1984-153233

19840725

OTHER SOURCE(S):

CASREACT 105:42382

For diagram(s), see printed CA Issue. The title compound (I), useful as an epoxy resin hardener and material for AB elastomers, polyurethane paint, etc. (no data), was prepared by treating isophorone (II) with HCN in presence of diazabicycloalkenes III (n = 2-11, m = 2-6; both rings may have lower alkyl substituents). Thus, III was added dropwise to II containing 1,8-diazabicyclo[5.4.0]undecene with stirring at 110° for 3 h and the resulting mixture held at 110° for 1 h to give 96.5% I based on HCN.

ANSWER 24 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1982:615625 CAPLUS

DOCUMENT NUMBER:

97:215625

TITLE:

GΙ

3-Cyano-3,5,5-trimethylcyclohexanone Nitto Chemical Industry Co., Ltd., Japan

PATENT ASSIGNEE(S):

Jpn. Kokai Tokkyo Koho, 4 pp.

SOURCE:

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICAT	ON NO. DATE
JP 57116038	A2	19820719	JP 1981-2	2102 19810112
JP 62005418	B4	19870204		
PRIORITY APPLN. INFO.	:		JP 1981-2102	19810112

AB3-Cyano-3,5,5-trimethylcyclohexanone (I) was prepared by reaction of isophorone (II) with HCN at 50-150° in the presence of bases and glycols. Thus, 27.5 parts HCN was added to a mixture of II 351.5, Na2CO3 2.7, and (HOCH2)2 25 parts over 3 h at 100° to give, after 0.5 h, 92.9% I.

ANSWER 25 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 1982:597874 CAPLUS

DOCUMENT NUMBER:

97:197874

TITLE:

A novel conjugate hydrocyanation with titanium tetrachloride-tert-butyl isocyanide

AUTHOR(S):

Ito, Yoshihiko; Kato, Hidehito; Imai, Hiroshi;

Saegusa, Takeo

CORPORATE SOURCE:

SOURCE:

Fac. Eng., Kyoto Univ., Kyoto, 606, Japan

Journal of the American Chemical Society (1982),

104(23), 6449-50

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: LANGUAGE:

Journal English

OTHER SOURCE(S):

CASREACT 97:197874

Conjugate hydrocyanation of $\alpha,\beta\text{-unsatd}.$ ketones is achieved in high yields by means of Me3CNC with TiCl4. Stereochem. of the conjugate hydrocyanation, which seems to be kinetically controlled, is demonstrated by the reactions of $\Delta 4(10)$ -octalin-3-one and 9-methyl- $\Delta 4(10)$ octalin-3-one with TiCl4-Me3CNC, producing a 9:1 mixture of trans- and cis-10-cyanooctalin-3-one and a 7:3 mixture of trans- and cis-10-cyano-9-methyloctalin-3-one, resp. The conjugate hydrocyanation may be explained in terms of nucleophilic β -addition of Me3CNC onto enone activated by TiCl4, followed by β -elimination of tert-Bu cation to give β-cyanoketone. Conjugate hydrocyanations of α,β -unsatd. aldehyde and ester are also achieved in moderate yields by EtAlCl2-Me3CNC system and AlCl3-Me3CNC system, resp.

ANSWER 26 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1981:514904 CAPLUS

DOCUMENT NUMBER: INVENTOR(S):

95:114904

TITLE:

3-Cyano-3,5,5-trimethylcyclohexanone

Dubreux, Bernard

PATENT ASSIGNEE(S):

Produits Chimiques Ugine Kuhlmann, Fr.

SOURCE:

Eur. Pat. Appl., 10 pp. CODEN: EPXXDW

DOCUMENT TYPE:

LANGUAGE:

Patent

French

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PA'	TENT NO.	K	IND	DATE		APPLICATION NO.	DATE
EP	28179		A1	19810506		EP 1980-401455	19801010
EP	28179		B1	19821103			
	R: AT,	BE, CH	, DE,	FR, GB,	IT, L	U, NL, SE	
FR	2468584		A1	19810508		FR 1979-26596	19791026
FR	2468584		В1	19840511			
US	4299775		A	19811110		US 1980-185989.	19800910
JP	56071057		A2	19810613		JP 1980-133078	19800926
JP	01047459	1	B4	19891013			
AΤ	1746		E	19821115		AT 1980-401455	19801010
ES	496269		A1	19811001		ES 1980-496269	19801024
PRIORIT	Y APPLN.	INFO.:			FR	1979-26596	19791026
					EP	1980-401455	19801010
				-			_

AB Isophorone reacted with metal cyanides and phase transfer agents to give the title compound (I). Thus, isophorone was heated with NaCN and Me(CH2)11N+(CH2Ph)Me2 Br- in water to yield I.

ANSWER 27 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1981:138907 CAPLUS

DOCUMENT NUMBER:

94:138907

10/458135

Page 22

- Same

TITLE:

Stereochemistry. LII. Orbital verification of reaction stereochemistry. III. The effects of

 β -fluoro and β -cyano groups on the

stereochemistry and kinetics of the reduction of cyclohexanones by lithium tri-tert-butoxyaluminum

hydride

AUTHOR (S):

Agami, C.; Kazakos, A.; Levisalles, J.; Sevin, A. Lab. Chim. Org., Univ. Paris VI, Paris, 5, Fr.

CORPORATE SOURCE: SOURCE:

Tetrahedron (1980), 36(20-21), 2977-81

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE:

French

LANGUAGE:

The effects were studied of $\beta\text{-fluoro}$ and $\beta\text{-cyano}$ groups on the

kinetics and stereoselectivity of the reduction of ketones by Li(Me3CO)3AlH in the presence of and absence of cryptands, Me(CH2)7F, and MeCN. The results were discussed in relation to ab initio MO calcns. on the analogous carbonyl compds., H2CRCH2CH0 (R = H, F, CN).

L8ANSWER 28 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1966:447345 CAPLUS

DOCUMENT NUMBER:

65:47345

ORIGINAL REFERENCE NO.:

65:8793d Synthesis of 3-cyano-3,5,5-trimethylcyclohexanone

PATENT ASSIGNEE(S):

Scholven-Chemie A.-G.

SOURCE:

8 pp. Patent

DOCUMENT TYPE: LANGUAGE:

Unavailable

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

APPLICATION NO. DATE PATENT NO. KIND DATE DATE _____ ____ _____ 19660425

NL 6513694

NL

PRIORITY APPLN. INFO.:

DE

The title compound (I) can be prepared batch-wise or continuously from isophorone, HCN, and 10-1-10-3% alkaline catalyst at 110-200°. Thus, a mixture of 50 l. isophorone, 20 l. HCN, and 280 ml. 15% NaOH in MeOH is heated to 150°, 12.5 l. HCN is added in 4 hrs., and the mixture stirred 0.5 hr., washed with 0.65% HNO3 solution to remove the alkaline catalvst,

and distilled to yield 10.3 kg. isophorone, 96.2% I, and 1.6 kg. residue. A detailed description of a continuous process is given.

=> d L9 1-7 ibib abs

ANSWER 1 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2004:386596 CAPLUS

DOCUMENT NUMBER:

140:391385

TITLE:

Regioselective hydrocyanation process for the calcium

oxide-catalyzed preparation of isophorone nitrile from

hydrogen cyanide and isophorone

INVENTOR(S):

Kunsmann-Keitel, Dagmar; Braun, Gerold; Muenster,

Ingo; Mundinger, Klaus; Scherhag, Gunter; Siegel,

Wolfgang

PATENT ASSIGNEE(S):

BASF Aktiengesellschaft, Germany

Eur. Pat. Appl., 5 pp. SOURCE: CODEN: EPXXDW

DOCUMENT TYPE:

Patent

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LANGUAGE:
                          German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:
     PATENT NO.
                     KIND DATE
                                           APPLICATION NO. DATE
     EP 1418172 A2 20040512 EP 2003-25652 20031107
     EP 1418172
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     DE 10251680 A1 20040519 DE 2002-10251680 20021107
JP 2004155785 A2 20040603 JP 2003-375444 20031105
     US 2004092761
                      A1 20040513
                                            US 2003-701513
                                        DE 2002-10251680 A 20021107
PRIORITY APPLN. INFO.:
     A regioselective hydrocyanation process for the calcium oxide-catalyzed
     preparation of isophorone nitrile from hydrogen cyanide and
     isophorone is presented in which the calcium oxide regioselective
     hydrocyanation catalyst has a BET surface area of >1.5 m2/g.
     ANSWER 2 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:
                          2000:96029 CAPLUS
DOCUMENT NUMBER:
                          132:124501
TITLE:
                          Hydrocyanation process and catalyst for the
                          preparation of 3-cyano-3,5,5-trimethylcyclohexanone
                          from isophorone and hydrogen cyanide
                          Fischer, Jakob; Siegel, Wolfgang; Bomm, Volker; Fischer, Martin; Mundinger, Klaus
INVENTOR (S):
                          BASF A.-G., Germany
PATENT ASSIGNEE(S):
SOURCE:
                          U.S., 4 pp.
                          CODEN: USXXAM
DOCUMENT TYPE:
                          Patent
LANGUAGE:
                          English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:
                  KIND DATE
     PATENT NO.
                                           APPLICATION NO. DATE
     US 6022988 A 20000208
DE 19836474 A1 20000217
                                            _____
                                            US 1999-372062
                                                              19990811
                                            DE 1998-19836474 19980812
     EP 985659 A1 20000315
EP 985659 B1 20031029
                                            EP 1999-115469
                                                             19990805
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO PRIORITY APPLN. INFO.:
                                         DE 1998-19836474 A 19980812
     3-Cyano-3,5,5-trimethylcyclohexanone is prepared in high yield and
     selectivity by reacting isophorone with hydrogen cyanide
   At 80-220° in the presence of the betaine catalyst
    /1,3-dimethylimidazolium-4-carboxylate.
REFERENCE COUNT:
                                THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS
                         12
                                RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
     ANSWER/3 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:
                         1995:907770 CAPLUS
DOCUMENT NUMBER:
                          123:313436
TITLE:
                          Process for the preparation of 3-cyano-3,5,5-
```

INVENTOR(S):

trimethylcyclohexanone [isophorone nitrile]

Mundinger, Klaus; Laqua, Gerhard; Witzel, Tom; Merger,

CODEN: EPXXDW

DOCUMENT TYPE:

Patent German

Α

LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

P	ATENT NO.	KIND DATE	APPLICATION NO.	DATE
_				
E	P 671384	A1 1995)913 B1 19991103	EP 1995-102923	19950302
E	P 671384	B1 19991103		
	R: BE, DE,	FR, GB		
D	E 4407487	Al 19950914	DE 1994-4407487	19940307

US 5516928 PRIORITY APPLN. INFO.:

DE 1994-4407487

US 1995-395322

19950228

CASREACT 123:313436; MARPAT 123:313436 OTHER SOURCE(S): GI

19960514

Me

Me

I

The title compound (I), an intermediate for the monomer isophoronediamine, is prepared by a method using improved catalysts. Thus, isophorone (II) reacts with HCN to give I, at 80-180° and 0.5-20 bar, in the presence of an ammonium salt catalyst R1R2R3R4N+ X- [R1-R4 = C1-18 alkyl, C5-8 cycloalkyl, aryl, C7-18 aralkyl, C2-18 hydroxyalkyl; X = 0C02H, or OC02R4 where R4 = C1-8 alkyl]. For example, a mixture of 3 mol HCN and 1.5 mol II was added over 60 min to a mixture of 4.5 mol II and 30 mmol Me4N+ MeOCO2- at 120°. Acidification with 3.5 g 85% H3PO4 and distillation at 0.1 mbar gave I in 99% or 96.2% yield (based on unreacted II or fed HCN, resp.). In comparison, use of Et4N+CN- catalyst gave 89.6% yield based on fed HCN. Also used as catalysts were BuMe3N+ MeOCO2-, and Et3MeN+ MeOCO2-, which gave similar results.

ANSWER 4 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN L9

ACCESSION NUMBER:

1994:511943 CAPLUS

DOCUMENT NUMBER:

121:111943

TITLE:

Purification of 3-cyano-3,5,5-trimethyl-1-

cyclohexanone

INVENTOR(S):

Terasawa, Shoichi; Yamamoto, Masahiro Asahi Chemical Ind, Japan

PATENT ASSIGNEE(S): SOURCE:

Jpn. Kokai Tokkyo Koho, 7 pp. CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06065183	A2	19940308	JP 1992-225631	19920825

```
JP 1992-225631
                                                               19920825
PRIORITY APPLN. INFO.:
     The title compound (I), prepared by the base-catalyzed addition reaction of HCN with isophorone, is purified by adding an inert compound having
     a higher b.p. than I and compatible with I, removing the basic catalyst,
     high-boiling impurities, and the inert compound in a thin-film evaporator,
     and separating isophorone from I in a distillation column. A reaction product
(180
     g) containing isophorone 18.02, I 80.9, high-boiling impurities 1.0, and NaOH
     0.08% was mixed with 3 g polyethylene glycol (II; mol. weight 400) and fed to
     a thin-film evaporator to give 177.3 g fraction containing 18.2% isophorone
     and 81.8% I (for separation by distillation) and 5.7 g fraction containing II
53,
     isophorone 3, and I 10%.
     ANSWER 5 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN
                          1994:511942 CAPLUS
ACCESSION NUMBER:
DOCUMENT NUMBER:
                          121:111942
                          Purification of 3-cyano-3,5,5-trimethyl-1-
TITLE:
                          cyclohexanone
                          Terasawa, Shoichi; Kondo, Yoshikimi
INVENTOR(S):
                          Asahi Chemical Ind, Japan
PATENT ASSIGNEE(S):
                          Jpn. Kokai Tokkyo Koho, 4 pp.
SOURCE:
                          CODEN: JKXXAF
DOCUMENT TYPE:
                          Patent
                          Japanese
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
     PATENT NO.
                     KIND DATE
                                           APPLICATION NO. DATE
                                        JP_06065182 A2 19940308
     JP 06065182 A2 19940308 JP 1992-215834 19920813
RITY APPLN. INFO.: JP 1992-160927 19920619
The title compound (I), prepared by the alkali-catalyzed addition reaction of
PRIORITY APPLN. INFO.:
     HCN with isophorone is purified by neutralizing the catalyst with
     an acid and distilling the mixture A reaction mixture containing I 60.5,
isophorone
     38, and KOH 0.30 mol was neutralized with H2SO4 and distilled (540 parts) in
     vacuo to give 226 parts distillate containing 12.7% I and 87.3% isophorone and
     286 parts crystalline fraction containing 99.5% I.
     ANSWER 6 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN
                          1993:670685 CAPLUS
ACCESSION NUMBER:
DOCUMENT NUMBER:
                          119:270685
                          Process for the continuous preparation of
TITLE:
                          3-cyano-3,5,5-trimethylcyclohexanone
                          Pander, Hans Joachim; Siegel, Hardo; Woerz, Otto
INVENTOR(S):
                          BASF A.-G., Germany
PATENT ASSIGNEE(S):
                          Eur. Pat. Appl., 6 pp.
SOURCE:
                          CODEN: EPXXDW
                          Patent
DOCUMENT TYPE:
LANGUAGE:
                          German
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
                                             APPLICATION NO. DATE
     PATENT NO.
                   KIND DATE
     EP 554786 A1 19930811
EP 554786 B1 19951129
                                             _____
                                                               _____
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DE 1992-4203456
DE 4203456
                  A1
                       19930812
                                                        19920207
US 5254711
                                       US 1993-14171
                  Α
                       19931019
                                                        19930205
JP 06122667
                                       JP 1993-18562
                  A2
                       19940506
                                                        19930205
JP 3241472
                  B2
                       20011225
                                    DE 1992-4203456 A 19920207
```

PRIORITY APPLN. INFO.: DE 19 OTHER SOURCE(S): CASREACT 119:270685

AB The title process comprises condensation of isophorone with HCN in a 2-stage flow reactor system comprising an initial stage wherein complete mixing is provided and a second stage wherein mixing is suppressed. Thus, operation at 150° in both stages gave 96.5% the title compound

cat is

L9 ANSWER 7 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1993:652567 CAPLUS

DOCUMENT NUMBER:

119:252567

TITLE:

Process for the preparation of 3-cyano-3,5,5-

trimethylcyclohexanone

INVENTOR(S):

Woodbury, Richard P.; Thunberg, Jon C.; Vankouwenberg,

Steven P.; Begonis, Walter B.

PATENT ASSIGNEE(S):

Hampshire Chemical Corp., USA

SOURCE:

U.S., 10 pp. CODEN: USXXAM

DOCUMENT TYPE: LANGUAGE: Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
	US 5235089	A	19930810	US 1992-843867	19920227	
	AU 9333783	A1	19930902	AU 1993-33783	19930225	
	AU 660765	B2	19950706			
	CA 2090555	AA	19930828	CA 1993-2090555	19930226	
	EP 558332	A1	19930901	EP 1993-301451	19930226	
	EP 558332	B1	19960529			
	R: AT, BE,	CH, DE	, DK, ES, FR, C	GB, IT, LI, NL, PT	, SE	
	JP 06016612	A2	19940125	JP 1993-61314	19930226	
	AT 138642	\mathbf{E}	19960615	AT 1993-301451	19930226	
	ES 2088225	Т3	19960801	ES 1993-301451	19930226	
PRIO	RITY APPLN. INFO	. :	US	5 1992-843867	19920227	
AB The title process giving title compound with high yield and <u>lo</u> w impurity						
comprises reacting isophorone with HCN in the presence of LiCN						
	catalyst at 80-115° while maintaining the HCN at a					
	controlled rate (to prevent the generation of free LiOH, diisophorone, its					
	nitrile derivs., and HCN polymer); and adding an acid selected					

=> => d his

(FILE 'HOME' ENTERED AT 15:09:39 ON 17 JUN 2004)

FILE 'REGISTRY' ENTERED AT 15:10:00 ON 17 JUN 2004

L1 1 S ISOPHORONENITRILE/CN

L2 1 S ISOPHORONE/CN

the Li salt.

FILE 'CASREACT' ENTERED AT 15:13:02 ON 17 JUN 2004

LiCN

CaO

from malic acid, oxalic acid, sulfuric acid, and phosphoric acid to precipitate

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10/458135
                                                                                  Page 27
                 STRUCTURE UPLOADED
               0 S L3
L4
L_5
               0 S L3 FULL
     FILE 'CAPLUS' ENTERED AT 15:15:24 ON 17 JUN 2004
L6
              88 S LT)
L7
           2508 S 13
             28 S L6 AND L7
L8
L9
              18 S L8 AND (HCN OR HYDROGEN CYANIDE)
L10
               7 S L9 AND ?OXIDE
               (BET or Brunauer Emett Teller)
=> s L10 and
         13208 BET
          2375 BRUNAUER
            34 EMETT
         15732 TELLER
            24 BRUNAUER EMETT TELLER
                  (BRUNAUER (W) EMETT (W) TELLER)
1.11
              1 L10 AND (BET OR BRUNAUER EMETT TELLER)
=> d L11
     ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
T.11
     2004:386596 CAPLUS
NA
DN
     140:391385
TI
     Regioselective hydrocyanation process for the calcium oxide
     -catalyzed preparation of isophorone nitrile from hydrogen
     cyanide and isophorone
     Kunsmann-Keitel, Dagmar; Braun, Gerold; Muenster, Ingo; Mundinger, Klaus;
IN
     Scherhag, Gunter; Siegel, Wolfgang
PA
     BASF Aktiengesellschaft, Germany
     Eur. Pat. Appl., 5 pp.
SO
     CODEN: EPXXDW
DT
     Patent
     German
LA
FAN.CNT 1
     PATENT NO.
                       KIND DATE
                                            APPLICATION NO. DATE
                      ---
     EP 1418172
                      A2 20040512
                                             EP 2003-25652
                                                               20031107
PΙ
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     DE 10251680
                        A1
                             20040519
                                             DE 2002-10251680 20021107
                                             JP 2003-375444
     JP 2004155785
                             20040603
                                                               20031105
                        Α2
     US 2004092761
                        A1
                             20040513
                                             US 2003-701513
                                                               20031106
PRAI DE 2002-10251680 A
                             20021107
=> d L11 ibib abs
                    CAPLUS COPYRIGHT 2004 ACS on STN
L11 ANSWER 1 OF 1
ACCESSION NUMBER:
                          2004:386596 CAPLUS
DOCUMENT NUMBER:
                          140:391385
TITLE:
                          Regioselective hydrocyanation process for the calcium
                          oxide-catalyzed preparation of isophorone
                          nitrile from hydrogen cyanide and
                          isophorone
INVENTOR(S):
                          Kunsmann-Keitel, Dagmar; Braun, Gerold; Muenster,
                          Ingo; Mundinger, Klaus; Scherhag, Gunter; Siegel,
                          Wolfgang
```

PATENT ASSIGNEE(S):

BASF Aktiengesellschaft, Germany Eur. Pat. Appl., 5 pp.

SOURCE:

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

	PATENT NO.	KIND DAT	E A	PPLICATION NO.	DATE		
	EP 1418172	A2 2004	40512 E	P 2003-25652	20031107		
	R: AT, BE,	CH, DE, DK	, ES, FR, GB,	GR, IT, LI, LU,	NL, SE, MC, PT,		
	IE, SI,	LT, LV, FI	, RO, MK, CY,	AL, TR, BG, CZ,	EE, HU, SK		
	DE 10251680	A1 2004	40519 Di	E 2002-10251680	20021107		
	JP 2004155785	A2 2004	40603 JI	P 2003-375444	20031105		
	US 2004092761	A1 2004	40513 U	S 2003-701513	20031106		
PRIO	RITY APPLN. INFO	.:	DE 20	002-10251680 A	20021107		
AB A regioselective hydrocyanation process for the calcium oxide							
-catalyzed preparation of isophorone nitrile from hydrogen							
cyanide and isophorone is presented in which the calcium							
	oxide regioselective hydrocyanation catalyst has a BET						
	surface area of	$>1.5 \text{ m}^{2}/\text{g}$.	_				